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SAMPLE SEARCH INITIATED 14:06:52
SAMPLE SCREEN SEARCH COMPLETED -      4 TO ITERATE
100.0% PROCESSED       4 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

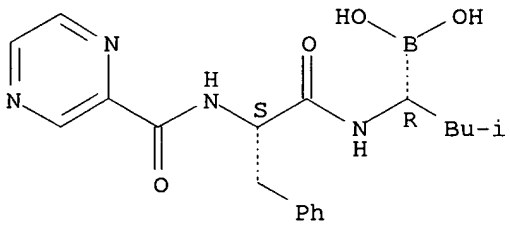
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            4 TO      200
PROJECTED ANSWERS:               1 TO       80

L2            1 SEA SSS SAM L1

=> d scan

L2   1 ANSWERS   REGISTRY  COPYRIGHT 1997 ACS
IN   Boronic acid, [3-methyl-1-[[1-oxo-3-phenyl-2-
     [(pyrazinylcarbonyl)amino]propyl]amino]butyl]-, [S-(R*,S*)]- (9CI)
MF   C19 H25 B N4 O4

Absolute stereochemistry.
```

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ALL ANSWERS HAVE BEEN SCANNED

=> s l1 full
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FULL SCREEN SEARCH COMPLETED -     64 TO ITERATE
100.0% PROCESSED      64 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.02

L3            3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             112.88     113.03

FILE 'CAPLUS' ENTERED AT 14:09:49 ON 25 APR 1997
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1997 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 25 Apr 1997  VOL 126 ISS 17
FILE LAST UPDATED: 25 Apr 1997  (970425/ED)

  To help control your online searching costs, consider using the
```

HCAplus file when using the FSEARCH command or when conducting SmartSELECT searches with large numbers of terms.

Some chemical substances have deleted CAS Registry Numbers. To ensure that you are using the most current CAS Registry Number, and for a more complete search, start your CAS Registry Number search in the REGISTRY file. Then use the L-number answer set from REGISTRY as a search term in CAplus.

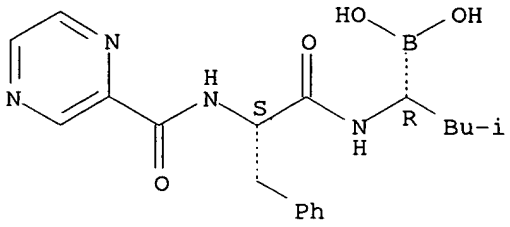
This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l3
L4            1 L3

=> d bib abs hitstr

L4   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 1997 ACS
AN   1996:466915  CAPLUS
DN   125:143315
TI   Boronic ester and acid compounds, synthesis and uses
IN   Adams, Julian; Ma, Yu-Ting; Stein, Ross; Baevsky, Matthew; Grenier,
     Louis; Plamondon, Louis
PA   Proscript, Inc., USA
SO   PCT Int. Appl., 144 pp.
     CODEN: PIXXD2
PI   WO 9613266 A1  960509
DS   W:  AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES,
         FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU,
         LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
         SI, SK
     RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR,
         IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI   WO 95-US14117  951027
PRAI US 94-330525  941028
     US 95-442581  950516
DT   Patent
LA   English
OS   MARPAT 125:143315
AB   Peptidyl boronic acids and esters PNR[B1R1X1]ACHR2X2CHR3BZ1Z2 [P =
     aryl-, aralkyl-, heteroaryl-, or heteroarylalkylcarbonyl or
     -sulfonyl; B1 = N, CH; X1, X2 = CONH, CH(OH)CH2, COCH2; A = 0, 1, 2;
     R = H, alkyl; RR1 or RR2 (for A = 0) may form a ring; R1, R2, R3 =
     H, alkyl, cycloalkyl, aryl, etc.; Z1, Z2 = alkyl, hydroxy, alkoxy,
     aryloxy; Z1Z2 may form a moiety derived from a dihydroxy compd.] and
     their pharmaceutically acceptable salts were prepd. The rate of
     degrdn. of proteins of an animal can be reduced by contacting cells
     of the animal with these boronic compds. Thus, N-(4-
     morpholinecarbonyl)-.beta.-(1-naphthyl)-L-alanine-L-leucine boronic
     acid was prepd. by coupling (1S,2S,3R,5S)-pinanediol leucine
     boronate trifluoroacetate salt with N-Boc-.beta.-(1-naphthyl)-L-
     alanine, followed by deprotection, acylation with
     4-morpholinecarbonyl chloride, and cleavage of the pinanediol
     moiety.
IT   179324-69-7 179324-85-7 179325-25-8
     RL: BAC (Biological activity or effector, except adverse); BIOL
```

(Biological study)
(synthesis of peptidyl boronic acids and esters as proteolytic enzyme inhibitors)

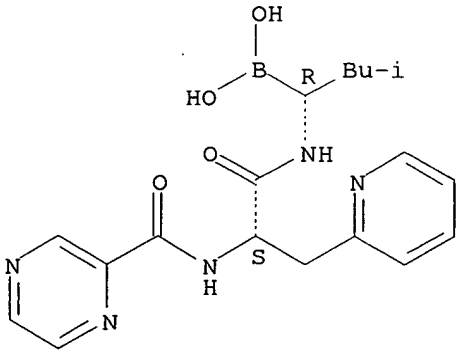
RN 179324-69-7 CAPLUS
CN Boronic acid, [3-methyl-1-[[1-oxo-3-phenyl-2-[(pyrazinylcarbonyl)amino]propyl]amino]butyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



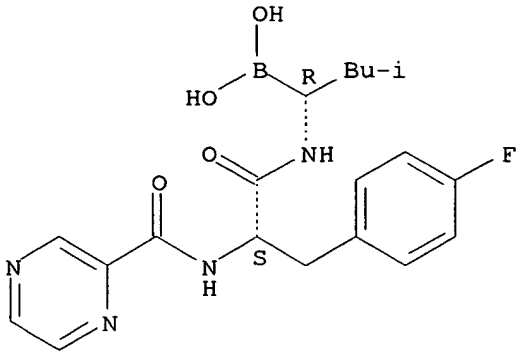
RN 179324-85-7 CAPLUS
CN Boronic acid, [3-methyl-1-[[1-oxo-2-[(pyrazinylcarbonyl)amino]-3-(2-pyridinyl)propyl]amino]butyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 179325-25-8 CAPLUS
CN Boronic acid, [1-[[3-(4-fluorophenyl)-1-oxo-2-[(pyrazinylcarbonyl)amino]propyl]amino]-3-methylbutyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=>
=> file beil

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.81	120.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.48	-0.48

FILE 'BEILSTEIN' ENTERED AT 14:17:56 ON 25 APR 1997
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FILE LAST UPDATED: 07 APR 1997

FILE COVERS 1779 TO 1996.
*** CAS REGISTRY NUMBERS FOR 4,355,851 SUBSTANCES AVAILABLE ***
*** FILE CONTAINS 7,000,722 SUBSTANCES ***

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* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
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=> d his

(FILE 'HOME' ENTERED AT 14:04:05 ON 25 APR 1997)

FILE 'REGISTRY' ENTERED AT 14:04:24 ON 25 APR 1997
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 3 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:09:49 ON 25 APR 1997
L4 1 S L3

FILE 'BEILSTEIN' ENTERED AT 14:17:56 ON 25 APR 1997

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SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE
100.0% PROCESSED       0 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            0 TO        0
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:19:50
FULL SCREEN SEARCH COMPLETED -      0 TO ITERATE
100.0% PROCESSED       0 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.05

L6            0 SEA SSS FUL L1

=> file marpat
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   0.00     120.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -0.48

FILE 'MARPAT' ENTERED AT 14:23:55 ON 25 APR 1997
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COPYRIGHT (C) 1997 American Chemical Society (ACS)

FILE CONTENT: 1988-PRESENT (VOL 104 ISS 14-VOL 126 ISS 16). (970418/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US   5610305  11 MAR 1997
DE  19535340  27 MAR 1997
EP    764630  26 MAR 1997
JP  09077771  25 MAR 1997
WO   9709453  13 FEB 1997

**Notice**  The first 1997 patent record appeared in MARPAT, with
            complete CA indexing and searchable Markush structure
            record, on 10 February 1997 -- US5591708 (970107),
            MARPAT 126:76542 -- just 5 weeks from issuance.

=> d his

     (FILE 'HOME' ENTERED AT 14:04:05 ON 25 APR 1997)
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     FILE 'REGISTRY' ENTERED AT 14:04:24 ON 25 APR 1997
L1                STRUCTURE UPLOADED
L2            1 S L1
L3            3 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 14:09:49 ON 25 APR 1997
L4            1 S L3

     FILE 'BEILSTEIN' ENTERED AT 14:17:56 ON 25 APR 1997
L5            0 S L1
L6            0 S L1 FULL

     FILE 'MARPAT' ENTERED AT 14:23:55 ON 25 APR 1997

=> s l3
SAMPLE SEARCH INITIATED 14:25:06
SAMPLE SCREEN SEARCH COMPLETED -      3 TO ITERATE
100.0% PROCESSED       3 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.11

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            3 TO      164
PROJECTED ANSWERS:               0 TO        0

L7            0 SEA SSS SAM L1

=> s l3 full
FULL SEARCH INITIATED 14:25:36
FULL SCREEN SEARCH COMPLETED -     77 TO ITERATE
100.0% PROCESSED      77 ITERATIONS  (     2 INCOMPLETE)        3 ANSWERS
SEARCH TIME: 00.00.18

L8            3 SEA SSS FUL L1

=> s l8 not l4
              1 L4
L9            2 L8 NOT L4

=> d bib abs qhit 1-2

L9   ANSWER 1 OF 2  MARPAT  COPYRIGHT 1997 ACS
(ALL HITs ARE ITERATION INCOMPLETES)
AN   125:143313  MARPAT
TI   Preparation of amidino and guanidino substituted peptide analogs as
     inhibitors of trypsin-like enzymes
IN   Lee, Sheng-lian O.; Carini, David John; Fevig, John Matthew;
     Kettner, Charles Adrian; Mantri, Padmaja; Feng, Zixia
PA   Du Pont Merck Pharmaceutical Company, USA
SO   PCT Int. Appl., 139 pp.
     CODEN: PIXXD2
PI   WO 9612499 A1  960502
DS   W:  AU, CA, JP, MX, NZ.
     RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI   WO 95-US13702  951024
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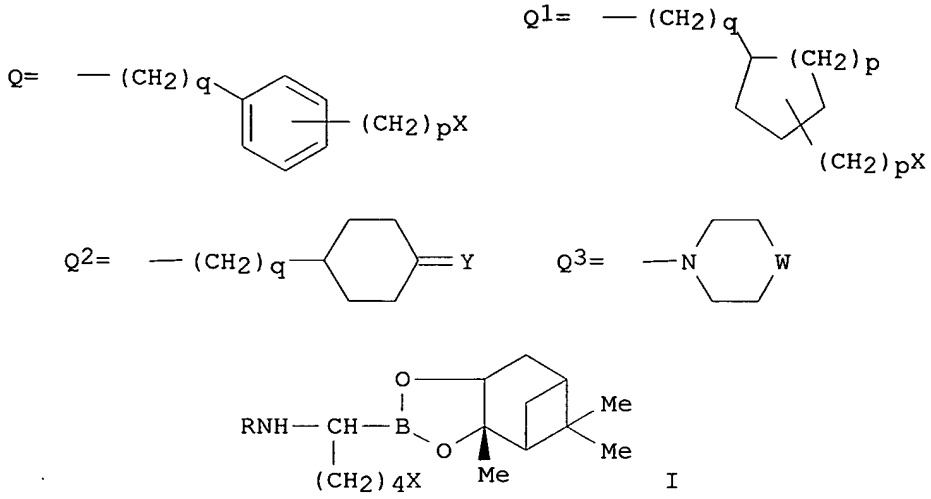
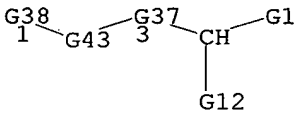
PRAI US 94-329039 941025
DT Patent
LA English
GI



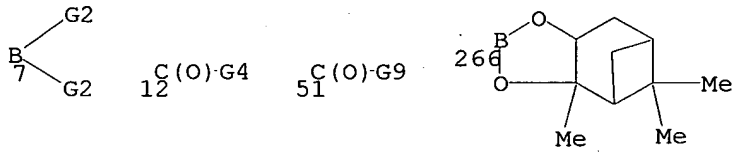
AB Novel .alpha.-aminoacid and .alpha.-aminoboronic acid and corresponding peptide analogs of formula R3[A]nNR2CHR1E [E = BY1Y2, COR14, CO2R4, CONR15R16, COR4, COCO2R4; wherein Y1, Y2 = OH, F, (un)substituted NH2; or Y1Y2 = cyclic boron ester, cyclic boron amide, or cyclic boron amide-ester contg. 2-20 carbon atoms and optionally 1-3 heteroatoms selected from N, S, and O; R4 = H, C1-4 alkyl, aryl-C1-4 alkyl, C5-7 cycloalkyl; R14 = CF3, CHF2, CH2F, CH2Cl, CO2R4, CONR15R16, COR4, etc.; R15, R16 = H, C1-4 alkyl, aryl-C1-4 alkyl, C5-7 cycloalkyl, (un)substituted Ph; or NR15R16 = Q3; wherein W = single bond, O, S, SO, SO2, CH2, NR4, NCOR4; R1 = (un)substituted C1-12 alkyl, Q, Q1; wherein X = halo, cyano, NO2, CF3, NH2, NHC(:NH)H, NHC(:NH)NHOH, NHC(:NH)NHCN, etc.; Y = O, :NOH, :NNHCHO; p = 0-3; q = 0-4; R2 = H, (un)substituted C1-12 alkyl, cycloalkyl, Ph, naphthyl, or aryl-C1-4 alkyl; R3 = H, alkyl, aryl, alkylaryl, S(O)rR7, COR7, CO2R7, P(O)2OR7, or any other C1-20 NH2-blocking group; wherein R7 = H, C1-4 alkyl, (un)substituted Ph, naphthyl, or aryl-C1-4 alkyl; r = 0-2; A = amino acid residue or peptide comprised of 2-20 amino acids residue; n = 0,1] and pharmaceutically acceptable salts thereof are prepd. These peptide analogs are useful for treating a physiol. disorder in a warm blooded animal catalyzed by trypsin-like enzymes, e.g. blood clotting, arterial thrombosis, myocardial infarction, inflammation, pancreatitis, and hereditary angioedema. Trypsin-like enzymes are a group of proteases which hydrolyze peptide bonds at basic residues liberating either a C-terminal arginyl or lysyl residue, among which are enzymes of the blood coagulation and fibrinolytic system required for hemostasis (e.g. factors II, X, VII, IX, kallikrein, tissue plasminogen activators, urokinase-like plasminogen activator, and plasmin), enzymes of the complement system, acrosin, and

pancreatic trypsin. Thus, Ac-D-Phe-Pro-OH was condensed with a boronic acid deriv. (I; R = H, X = Br) by a mixed anhydride procedure using iso-Bu chloroformate and N-methylmorpholine in CCl4 to give an intermediate I (R = Ac-D-Phe-Pro, X = Br), which was heated with Bu4NCN in MeCN at 90.degree. for 3 h to give the nitrile I (R = Ac-D-Phe-Pro, X = cyano). The latter nitrile was stirred with satd. methanolic HCl at 4.degree. overnight, concd., and redissolved in MeOH. NH3(g) was bubbled through the soln. for 1 h and the soln. was heated at 50.degree. for 3 h to give I [R = Ac-D-Phe-Pro, X = C(:NH)NH2]. This compd. in vitro inhibited thrombin with Ki of <500 nM.

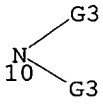
MSTR 1A ITERATION INCOMPLETE



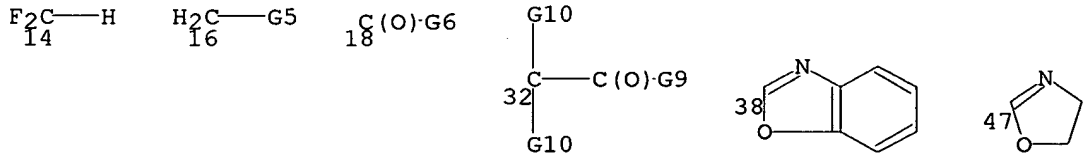
G1 = 7 / Hy<EC (3-6) Q (1) B (-5) N (-5) O (-3) S (0) OTHERQ (2-20) C, AN (1) B> / 12 / 51 / (SC 266)



G2 = OH / F / 10 / alkoxy<(1-8)>

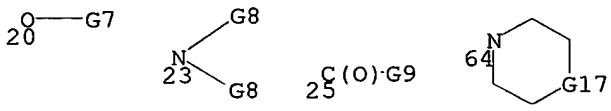


G3 = H / alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)>
G4 = CF3 / 14 / 16 / 18 / 32 / 38 / 47 / Hy<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1-3)> (SO) / 207

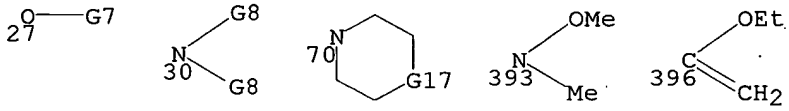


G44=O
207

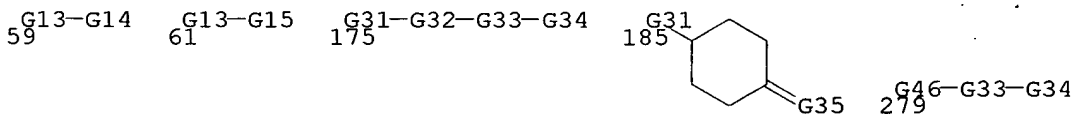
G5 = F / Cl / Br
G6 = OH / 20 / 23 / 64 / H / alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)> / 25

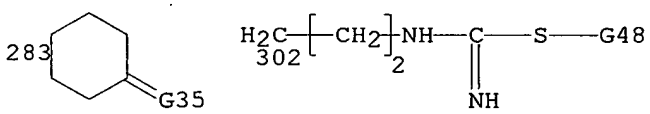


G7 = alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)>
G8 = H / alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)> / Ph (SO)
G9 = OH / 27 / 30 / 70 / H / alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)> / (SC 393 / 396)

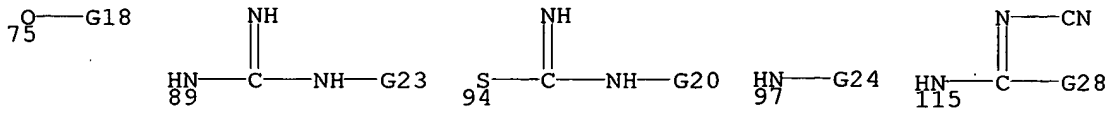


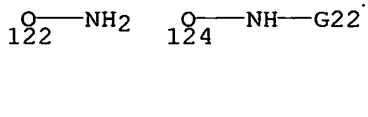
G10 = OH / H / F
G12 = 59 / 61 / 175 / 279 / 185 / 283 / (SC 302)

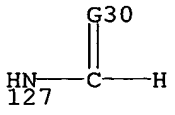


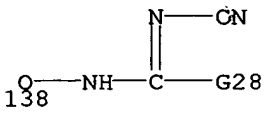


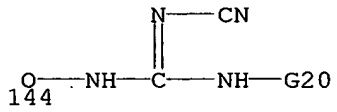
G13 = alkylene<(1-12)>
G14 = H / OH / 75 / 89 / 94 / 97 / 115 / 122 / 124 / 127 / 138 / 144 / 151 / 156 / 161 / 165

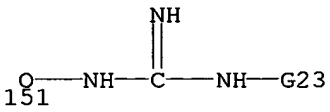


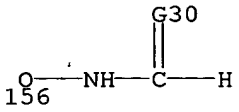


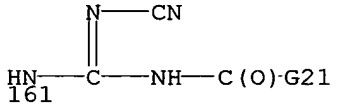


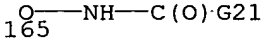




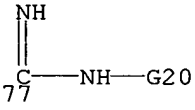




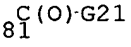




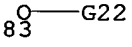
G15 = CN / 77



G16 = Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2), RS (1-2) E6 (0) OTHER> (SO)
G17 = O / S / S(O) / SO2 / NULL / CH2 / NH (SO)
G18 = alkyl<(1-12)> (SO) / cycloalkyl (SO) / Hy<EC (0-) O (0-) S (0-) N (0) OTHERQ, AR (0), BD (ALL) SE> (SO) / Ph (SO) / naphthyl (SO) / alkyl<(1-4)> (SR G19)
G19 = (1-) G16 / R
G20 = H / alkyl<(1-4)> (SO G16) / Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2), RS (1-2) E6 (0) OTHER> (SO) / 81

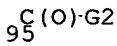


G21 = H / alkyl<(1-4)> (SO G16) / Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2), RS (1-2) E6 (0) OTHER> (SO) / OH / 83

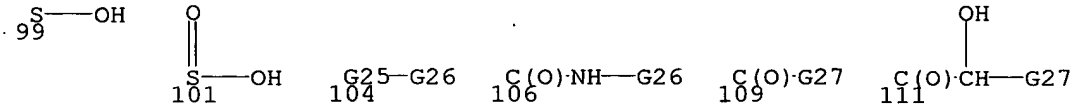


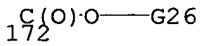
G22 = alkyl<(1-4)> (SO G16) / Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2),

RS (1-2) E6 (0) OTHER> (SO)
G23 = H / alkyl<(1-4)> (SO G16) /
Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2),
RS (1-2) E6 (0) OTHER> (SO) / OH / 95

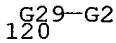


G24 = SH / 99 / 101 / 104 / CONH2 / 106 / 109 / 111 /
CO2H / 172

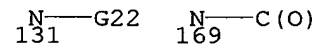




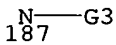
G25 = S / S(O) / SO2
G26 = alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)>
G27 = H / alkyl<(1-4)> (SO G16) / cycloalkyl<(5-7)>
G28 = SH / 120 / NH2



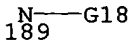
G29 = S / NH
G30 = NH / 131 / 169



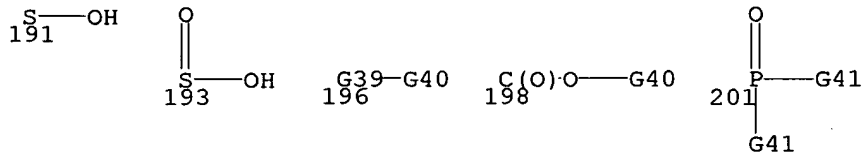
G31 = alkylene<EC (1-4) C, DC (0) M3>
G32 = phenylene / cycloalkylene<(4-7)>
G33 = NULL / alkylene<EC (1-3) C, DC (0) M3>
G34 = R / (SC C(NH)NH2 / CH2NH2 / Br / CN / NH2 / OH /
NHC(NH)NH2 / CO2Me)
G35 = O / 187

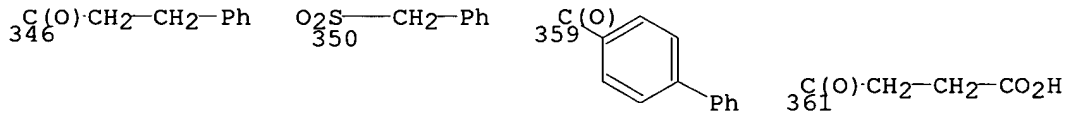


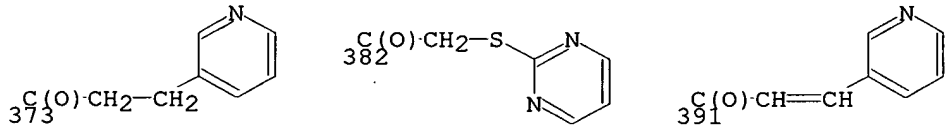
G36 = OH / NHCHO
G37 = NH / 189



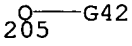
G38 = H / alkyl (SO G16) / Ph (SO) / naphthyl (SO) / SH / 191 / 193 / CHO / CO2H / 196 / 198 / 201 / (SC 346 / 350 / 359 / 361 / 373 / 382 / 391 / CO2CH2Ph / SO2Ph / CH2Ph / CH2CO2H)



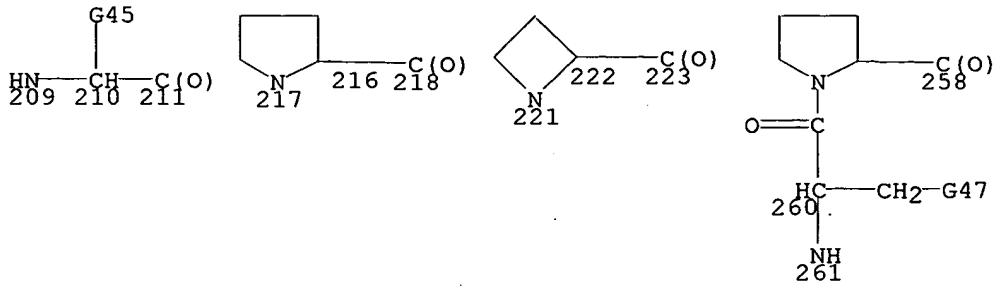


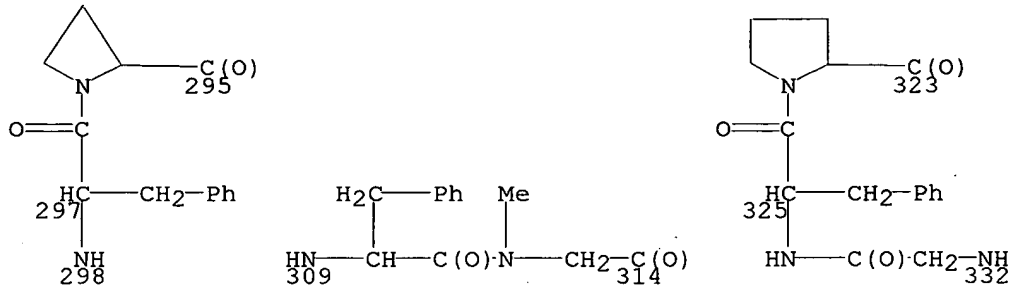


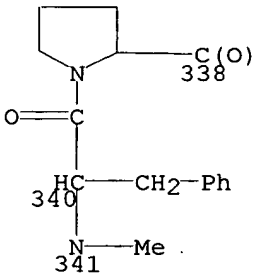
G39 = S / S(O) / SO2 / C(O)
G40 = H / alkyl (SO G16) / Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2), RS (1-2) E6 (0) OTHER> (SO)
G41 = OH / 205



G42 = alkyl (SO G16) / Ph (SO) / naphthyl (SO)
G43 = R<TX "peptide residue of 1-20 amino acids"> / (SC 209-1 211-3 / 217-1 218-3 / 221-1 223-3 / 261-1 258-3 / 298-1 295-3 / 309-1 314-3 / 332-1 323-3 / 341-1 338-3)

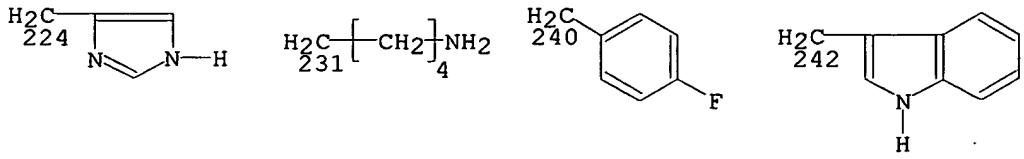






G44 = Hy<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1-3)> (SO)

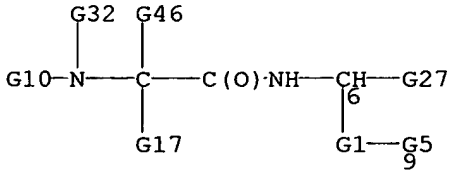
G45 = Me / CH2CH2CH2NHC(NH)NH2 / CH2CONH2 / CH2CO2H / CH2SH / CH2CH2CONH2 / CH2CH2CO2H / H / 224 / 231 / Bu-s / Bu-i / CH2CH2CH2CH2NH2 / CH2CH2SMe / CH2CH2CH2NH2 / CH2Ph / 240 / CH2OH / CH(OH)Me / 242 / CH2C6H4OH-p / Pr-i



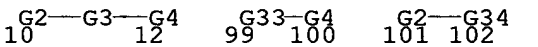
G46 = phenylene / cycloalkylene<(4-7)>
G47 = Ph / thiazolyl / 2-pyridyl / 3-pyridyl / 2-thienyl
G48 = CH2CH=CH2 / Me / Et
DER: and pharmaceutically acceptable salts
MPL: claim 1
NTE: substitution is restricted
NTE: alkyl groups in G18 may contain heteroatom interruptions
STE: 210,216,222 - D,L; 260,297 - D

L9 ANSWER 2 OF 2 MARPAT COPYRIGHT 1997 ACS
(ALL HITs ARE ITERATION INCOMPLETES)
AN 123:957 MARPAT
TI Electrophilic peptide analogs as inhibitors of trypsin-like enzymes
IN Galemmo, Robert Anthony, Jr.; Abelman, Matthew Mark; Amparo, Eugene Cruz; Fevig, John Matthew; Knabb, Robert Madara; Miller, William Henry; Pacofsky, Gregory James; Weber, Patricia Carol
PA Du Pont Merck Pharmaceutical Co., USA
SO PCT Int. Appl., 307 pp.
CODEN: PIXXD2
PI WO 9509634 A1 950413
DS W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, PL, SK
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 94-US11280 941006
PRAI US 93-133251 931007
US 93-139445 931020
DT Patent
LA English
AB Electrophilic dipeptide analogs R3R11NCR4R5C(O)NHCHR1A [R1 = ZX; Z = C1-12 alkyl or alkenyl, (CH2)qC6H4(CH2)p; p = 0-3; q = 0-4; X = halo, CN, NO2, CF3, NH2, etc.; R3 = C(O)Y; Y = aryl, aralkyl, heterocyclyl, heterocyclylalkyl, cycloalkylalkyl, adamantylalkyl, etc.; R4, R5 = H, C1-4 alkyl, (C1-4 alkyl)aryl, C5-7 cycloalkyl; R11 = C1-4 alkyl, C3-6 cycloalkyl, alkoxy, NH2, (di)alkylamino, aryl, heterocyclyl, etc.; A = B(OH)2, BF2, cyclic B ester or amide, C(O)CF3, C(O)C(O)NH2, CH(OH)(CH2F), etc.] in which an electrophilic deriv. of an .alpha.-amino acid is conjugated to an N,N-disubstituted .alpha.-amino acid are prepd. as inhibitors of trypsinlike serine proteases for use as antithrombotics. Thus, N-hydrocinnamoyl-N-(2,2-dimethyl-2-phenylethyl)glycylborolysine-HCl (I) was prepd. by condensation of H2NCH2C(O)OEt.HCl with PhCMe2CHO (prepn. given) followed by PhCH2CH2C(O)Cl and Br(CH2)4CH(NH2)B(OH)2 pinanediol ester and transesterification with PhB(OH)2. I showed Ki <500 nM for thrombin, Factor Xa, and Factor VIIa using synthetic chromogenic substrates and IC50 <500 nM for thrombin time.

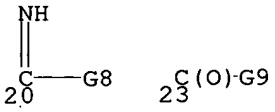
MSTR 1C ITERATION INCOMPLETE



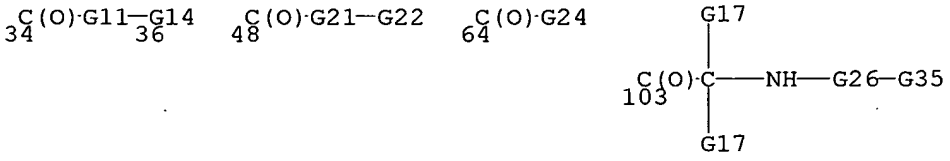
G1 = Ak<EC (1-12) C, BD (0-) D (0) T> / phenylene /
99-6 100-9 / 101-6 102-9 / 10-6 12-9

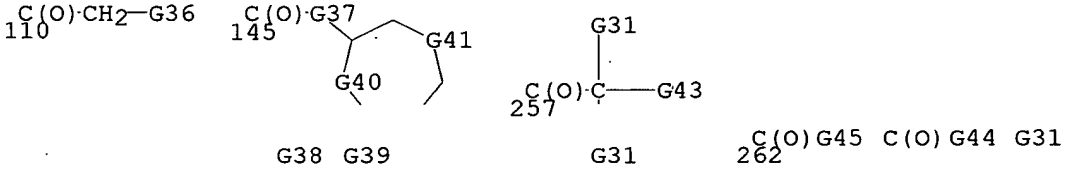


G2 = alkylene<(1-4)>
G3 = phenylene
G4 = alkylene<(1-3)>
G5 = CN / CF3 / 20 / 23



G8 = NH2 / alkylamino<(1-4)> / NHCHO /
alkylcarbonylamino<(1-4)>
G9 = NH2 / alkylamino<(1-4)> / OH / alkoxy<(1-4)>
G10 = 34 / 48 / 64 / 103 / 145 / 110 / 257 / 262 / 267





C(O)G45 C(O)G44 G31
267

G11 = NULL / alkylene (SO (-2) G12) / alkenylene<(2-5)> /
39-34 40-36 / 45-34 47-36

39 G15—G18 40 45 G18—G19—G20 47

G12 = alkoxy<(1-4)> / aryl<RC (1-3),
RS (0-1) E5 (1-2) E6 (0) OTHER> (SO) /
Hy<EC (1-2) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1-2),
RS (-1) E5 (-2) E6 (0) OTHER> (SO) /
aryloxy<RC (1-3), RS (0-1) E5 (1-2) E6 (0) OTHER> (SO) / 37

37 C(O)-G13

G13 = OH / alkoxy<(1-4)> (SO aryl<RC (1-3),
RS (0-1) E5 (1-2) E6 (0) OTHER> (SO)) / cycloalkyloxy<(5-7)>
G14 = aryl<RC (1-3), RS (0-1) E5 (1-2) E6 (0) OTHER>
(SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ,
RC (1-2), RS (-1) E5 (-2) E6 (0) OTHER> (SO)
G15 = O / S / S(O) / SO2 / 41

41 N——G16

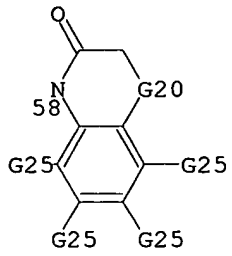
G16 = H / alkyl<(1-4)> (SO aryl<RC (1-3),
RS (0-1) E5 (1-2) E6 (0) OTHER> (SO)) / cycloalkyl<(5-7)> /
43

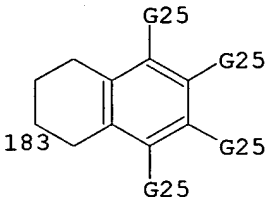
43 C(O)-G17

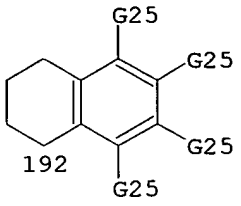
G17 = H / alkyl<(1-4)> (SO aryl<RC (1-3),
RS (0-1) E5 (1-2) E6 (0) OTHER> (SO)) / cycloalkyl<(5-7)>
G18 = CH2 (SO)
G19 = O / S / S(O) / SO2
G20 = (0-2) CH2
G21 = (1-3) CH2
G22 = adamantyl / cycloalkyl<(5-7)> / 51

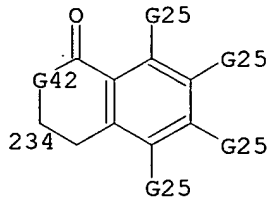
51 G42—G23

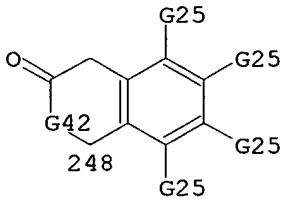
G23 = cycloalkyl<(5-7)>
G24 = Ph (SR) / 58 / 183 / 192 / 204 / 234 / 248



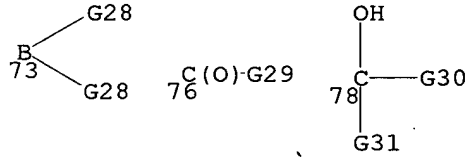




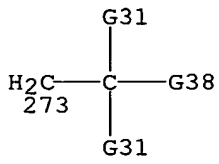


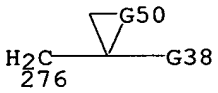


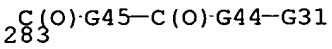
G25 = H / R
G26 = S / S(O) / SO2
G27 = 73 / Hy<EC (3-6) Q (1) B (0-) N (0-) O (0-3) S (0) OTHERQ (2-20) C> / 76 / 78

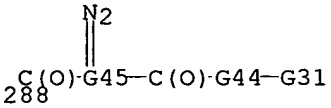


G28 = OH / F / NH2 (SO) / alkoxy<(1-8)>
G29 = R / (EX H)
G30 = R / (EX H)
G31 = H / R
G32 = alkyl<(1-4)> (SO aryl<RC (1-3), RS (0-1) E5 (1-2) E6 (0) OTHER> (SO)) / cycloalkyl<(3-6)> / OH (SO) / NH2 (SO) / CONH2 (SO) / aryl<RC (1-3), RS (0-1) E5 (1-2) E6 (-1) E7 (0) OTHER> (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1-2), RS (-1) E5 (-2) E6 (0) OTHER> (SO) / alkyl<(1-4)> (SR Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1-2), RS (-1) E5 (-2) E6 (0) OTHER> (SO)) / alkyl<(1-4)> (SR CO2H (SO)) / 273 / 276 / 283 / 288

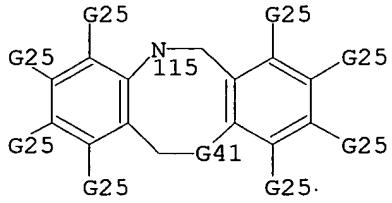


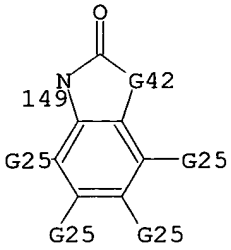


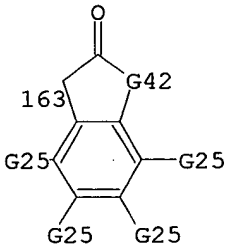


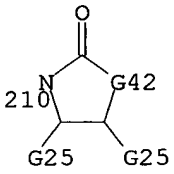


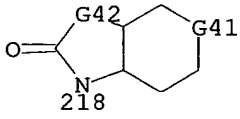
G33 = phenylene
G34 = phenylene
G35 = naphthyl (SO)
G36 = 115 / 149 / 163 / 210 / 218











G37 = (0-3) CH2
G38 = Ph (SO)
G39 = (0-4) CH2
G40 = (0-1) CH2
G41 = (0-2) CH2
G42 = O / S / S(O) / SO2 / NH (SO)
G43 = NH2 (SO)
G44 = O / NH
G45 = Ak<EC (3-) C, BD (ALL) SE> (SO)
G46 = H / alkyl<(1-4)> (SO aryl<RC (1-3), RS (0-1) E5 (1-2) E6 (0) OTHER> (SO)) / cycloalkyl<(5-7)>
G50 = alkylene
G32+G46= CH2CH2
DER: or pharmaceutically acceptable salts, hydrates or prodrugs
MPL: claim 1
NTE: additional ring formation allowed

```
NTE:     substitution is restricted


=>
=>
=> s l9/com
LIMIT NOT VALID FOR L9
This qualification can be applied only to a structure answer set
L-number.

=>
=> d his

     (FILE 'HOME' ENTERED AT 14:04:05 ON 25 APR 1997)

     FILE 'REGISTRY' ENTERED AT 14:04:24 ON 25 APR 1997
L1              STRUCTURE UPLOADED
L2            1 S L1
L3            3 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 14:09:49 ON 25 APR 1997
L4            1 S L3

     FILE 'BEILSTEIN' ENTERED AT 14:17:56 ON 25 APR 1997
L5            0 S L1
L6            0 S L1 FULL

     FILE 'MARPAT' ENTERED AT 14:23:55 ON 25 APR 1997
L7            0 S L3
L8            3 S L3 FULL
L9            2 S L8 NOT L4

=> s l8/com
L10           1 L8/COM

=> s l10 not l4
              1 L4
L11           0 L10 NOT L4

=>
=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      54.09     174.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -0.92      -1.40

STN INTERNATIONAL LOGOFF AT 14:35:48 ON 25 APR 1997
```